Propan-2-(^{17}O)ol
1173018-27-3 | DTXSID30745952

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 5.72e-12 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 7.36e-01

Confidence level: 6.66e-01

Nearest Neighbors from the Training Set

Image not found
Isopropanol
Measured: 5.07e-12
Predicted: 5.72e-12

Image not found
1-Propanol
Measured: 5.53e-12
Predicted: 7.35e-12

Image not found
1,4-Diazabicyclo[2.2.2]octane
Measured: 2.20e-11
Predicted: 1.30e-11

Image not found
Diethyl ether
Measured: 1.31e-11
Predicted: 9.74e-12

Image not found
tert-Butyl alcohol
Measured: 1.12e-12
Predicted: 3.20e-12